MCNPX: Accomplishments and Possibilities

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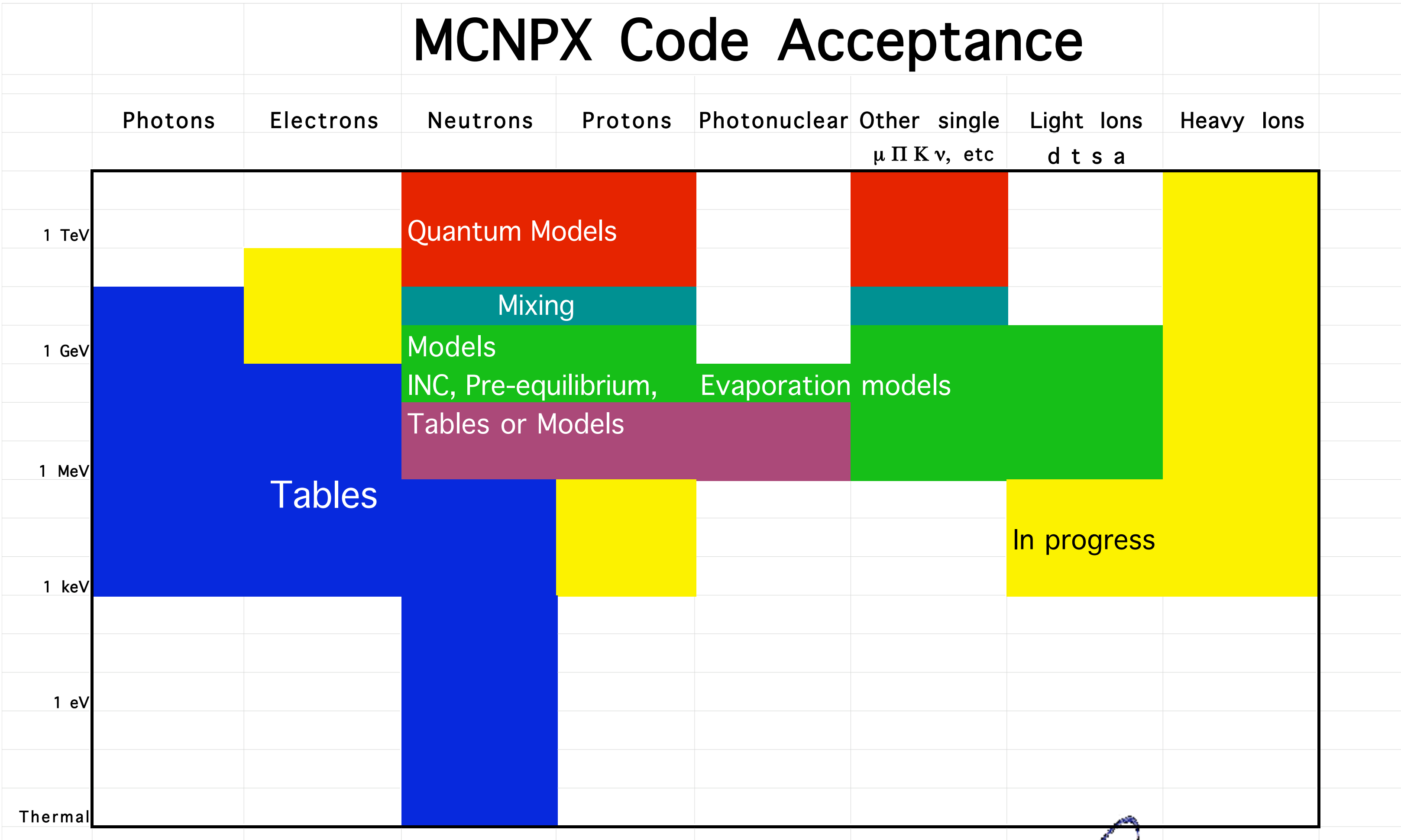
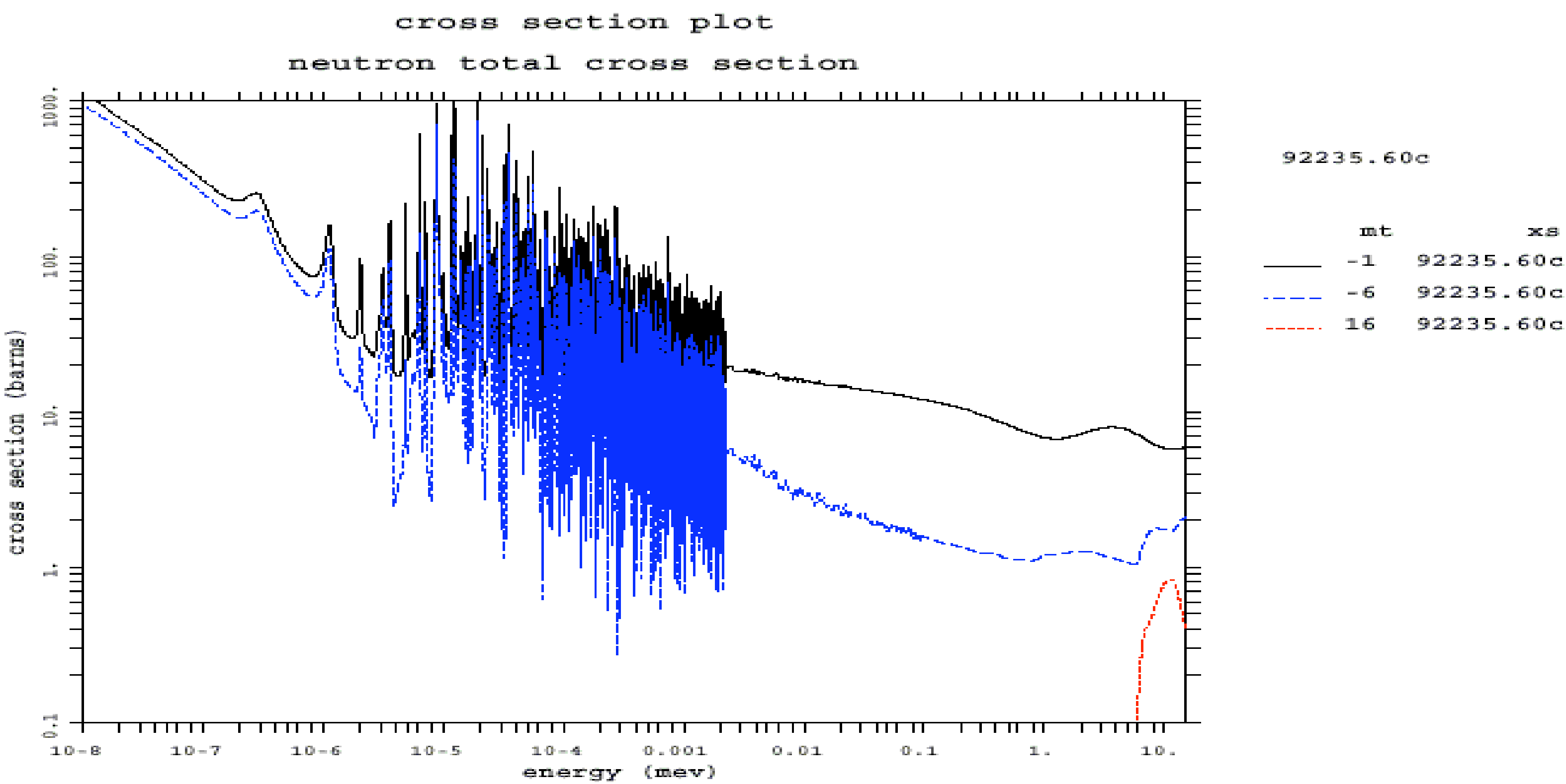
MCNPX: Monte Carlo N-Particle eXtended

MCNP4C3 Extended to nearly all particles, energies, applications



MCNPX: Monte Carlo N-Particle eXtended

Continuous energy, 3D, time-dependent



MCNPX: Accomplishments and Possibilities

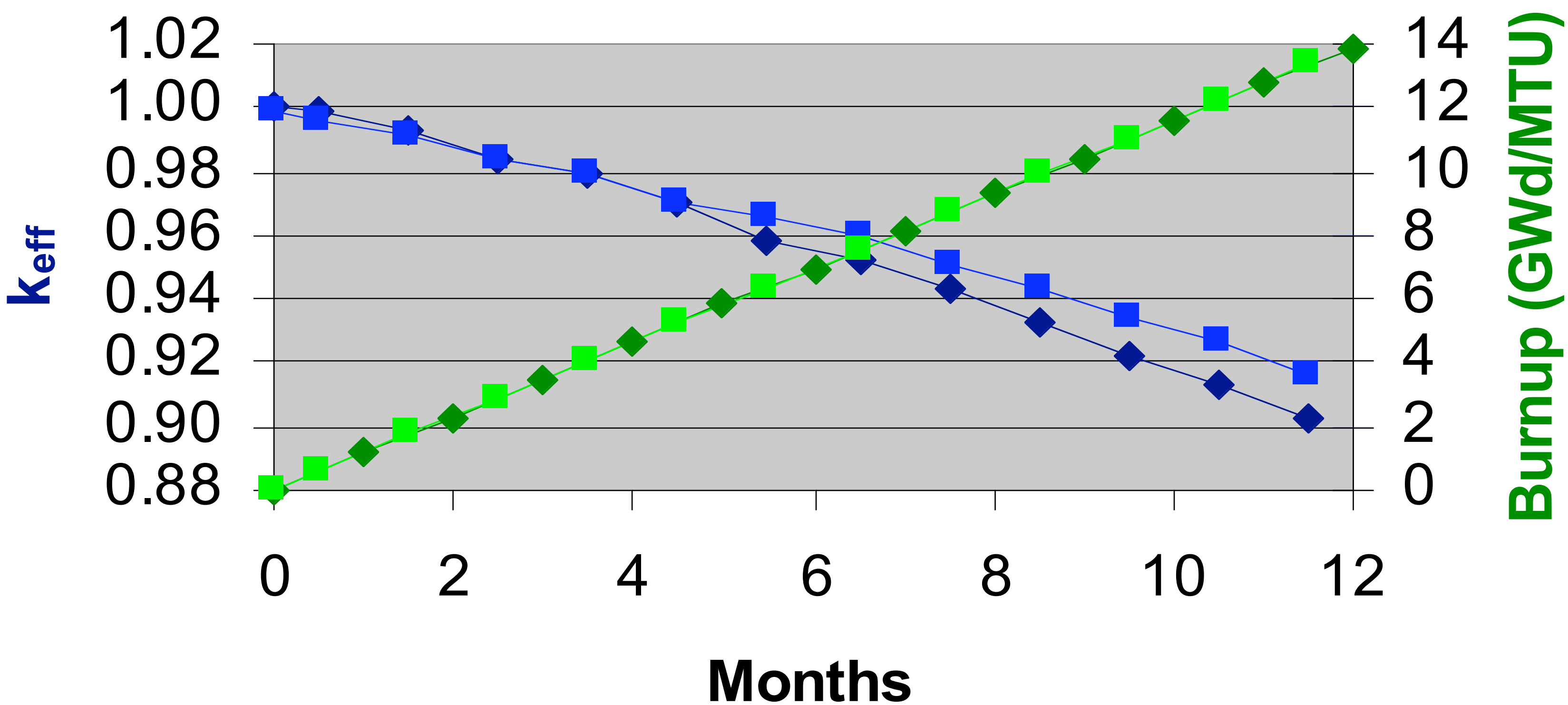
FY05 Accomplishments

- Integration of CINDER90 into MCNPX (2)
- Mesh Tally Plots Superimposed on Geometry (3)
- Correct Flux Distributions in Near-Critical Systems
- Ongoing
  - INCL upgrade
  - Maintenance
  - Documentation
  - User support / training
  - SQA / modernization

0.7 FTE

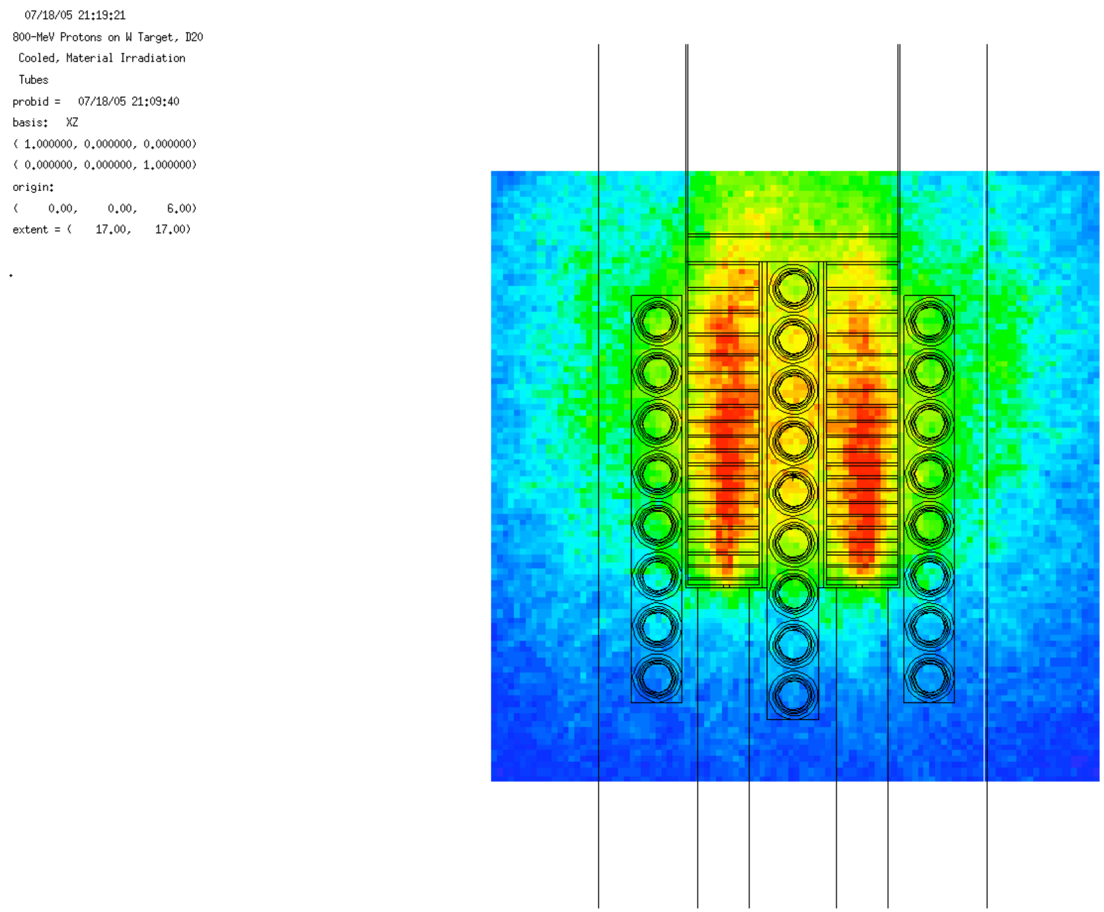
MCNPX: Accomplishments and Possibilities

FY05: Integration of CINDER90 into MCNPX (2)



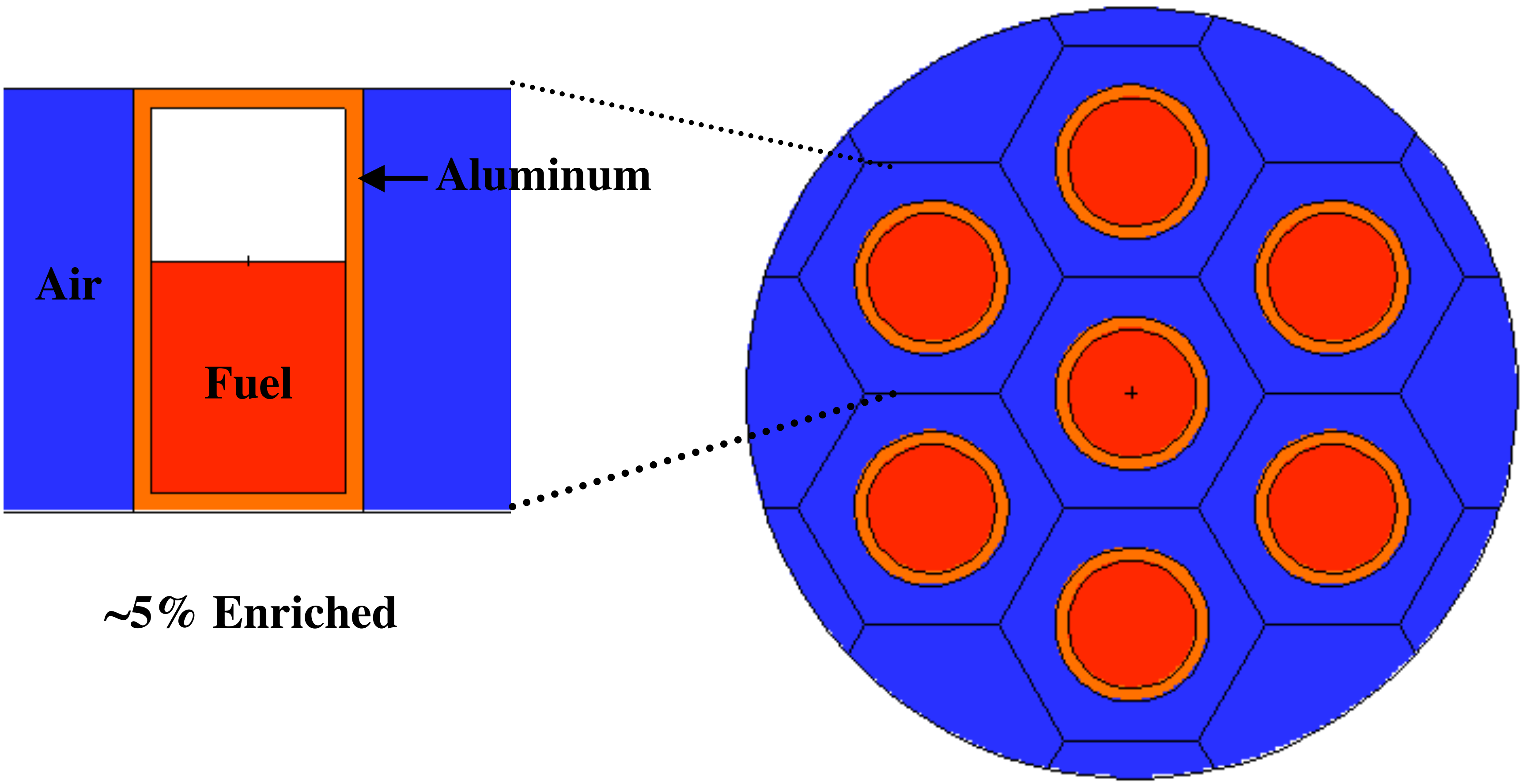
MCNPX: Accomplishments and Possibilities

FY05: Mesh Tally Plots Superimposed on Geometry (3)



Purdue Collaboration: Correct Estimate of Fluxes

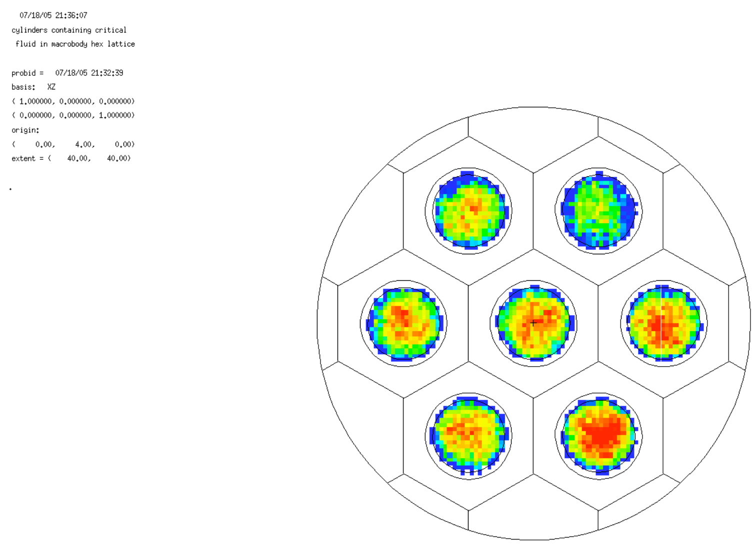
7-Can HEU Test Problem

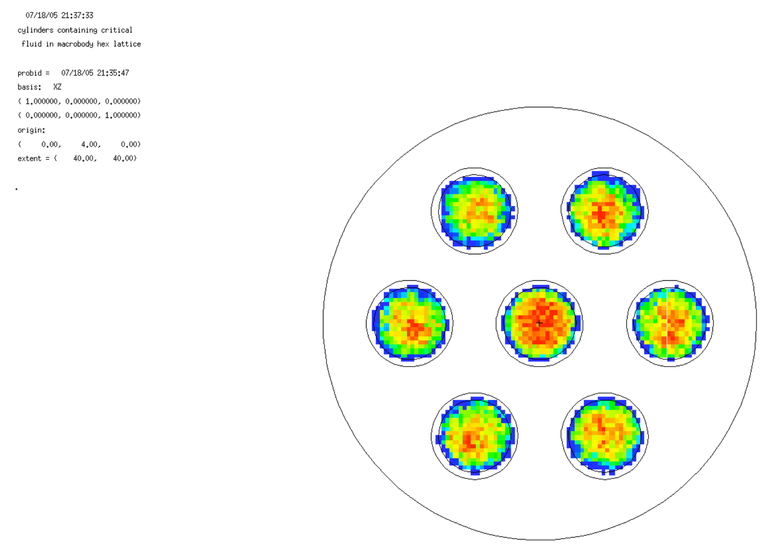


~5% Enriched

MCNPX: Accomplishments and Possibilities

FY05: Correct Flux Distributions in Near-Critical Systems





Standard Monte Carlo

Vacation Matrix Method

MCNPX: Accomplishments and Possibilities

FY05 Accomplishments:

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MCNPX: Accomplishments and Possibilities
FY06 Milestones:

- AFCI: Implement predictor/corrector step for CINDER'90 burnup module in MCNPX *0.25 FTE*
    - code maintenance / documentation;
    - release of code versions with new capabilities / SQA;
    - user training / workshops / support;
    - research into correct flux / source distributions in near-critical systems in collaboration with Purdue University.
- MTS: CEM03 / LAQGSM *0.4 FTE*
- GEN-IV: none
- Other: MCNPX/MCNP merger

MCNPX Depletion Capability

- Steady State Monte Carlo (MCNPX) linked Depletion (CINDER90)
- Allows complete, relatively easy-to-use depletion calculations in a single Monte Carlo code
- User input and Top level processing is minimized
  - Eliminates cumbersome input files and complex directory structures
- Available time dependant results
  - Burnup
  - Eigenvalue
  - Isotope Concentrations
  - System Flux
  - System Average v and Q

```
...
C  Control Cards
vol   192.287
kcode  5000 1.0 5 300
ksrc  0.65665 0.65665 150.0
BURN  TIME=0.645,40,100,140,200,250
      MAT=1
      POWER=0.066956
      PFRAC=1.0,1.0,1.0,1.0,1.0,1.0
      OMIT=1,8,6014,7016,8018,9018,90234,91232,95240,95244
      BOPT=1.0, -14
C  Material Cards
m1
      8016.60c   4.5854e-2
      92235.60c  1.4456e-4
      92238.60c  1.9939e-2
      94238.60c  1.1467e-4
      94239.60c  1.0285e-3
      94240.60c  7.9657e-4
      94241.60c  3.3997e-4
      94242.60c  5.6388e-4
...
```

Total Depletion Input

Organized Easy-to-Understand Output

- Available time dependant system averaged results
  - Burnup
  - Eigenvalue
  - Isotope Concentrations
  - System Flux
  - System Average ν and Q
- Available time dependant individual burn material results results
  - Burnup
  - Isotope Concentrations

...

step	duration (days)	time (days)	power (MW)	keff	flux	ave. nu	ave. q	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	1.000E+00	1.15793	4.428E+15	2.878	209.106	0.000E+00
1	1.000E+02	1.000E+02	1.000E+00	1.14188	4.499E+15	2.877	209.099	5.734E+01
2	7.000E+01	1.700E+02	1.000E+00	1.15781	4.408E+15	2.877	209.100	9.747E+01

...

...

Individual Material Burnup

Material #: 1

step	duration (days)	time (days)	power fraction	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	1.000E+02	1.000E+02	1.000E+00	5.734E+01
2	7.000E+01	1.700E+02	1.000E+00	9.747E+01

...

...

actinide inventory for material 1 ...

no.	zaid	mass (gm)	activity (Ci)	spec.act. (Ci/gm)	atom den. (a/b-cm)	atom fr.	mass fr.
1	92235	1.085E+01	0.000E+00	0.000E+00	1.446E-04	6.305E-03	6.219E-03
2	92234	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

...

nonactinide inventory for material 1 ...

no.	zaid	mass (gm)	activity (Ci)	spec.act. (Ci/gm)	atom den. (a/b-cm)	atom fr.	mass fr.
1	8016	2.342E+02	0.000E+00	0.000E+00	4.585E-02	1.000E+00	1.000E+00
2	8017	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

...

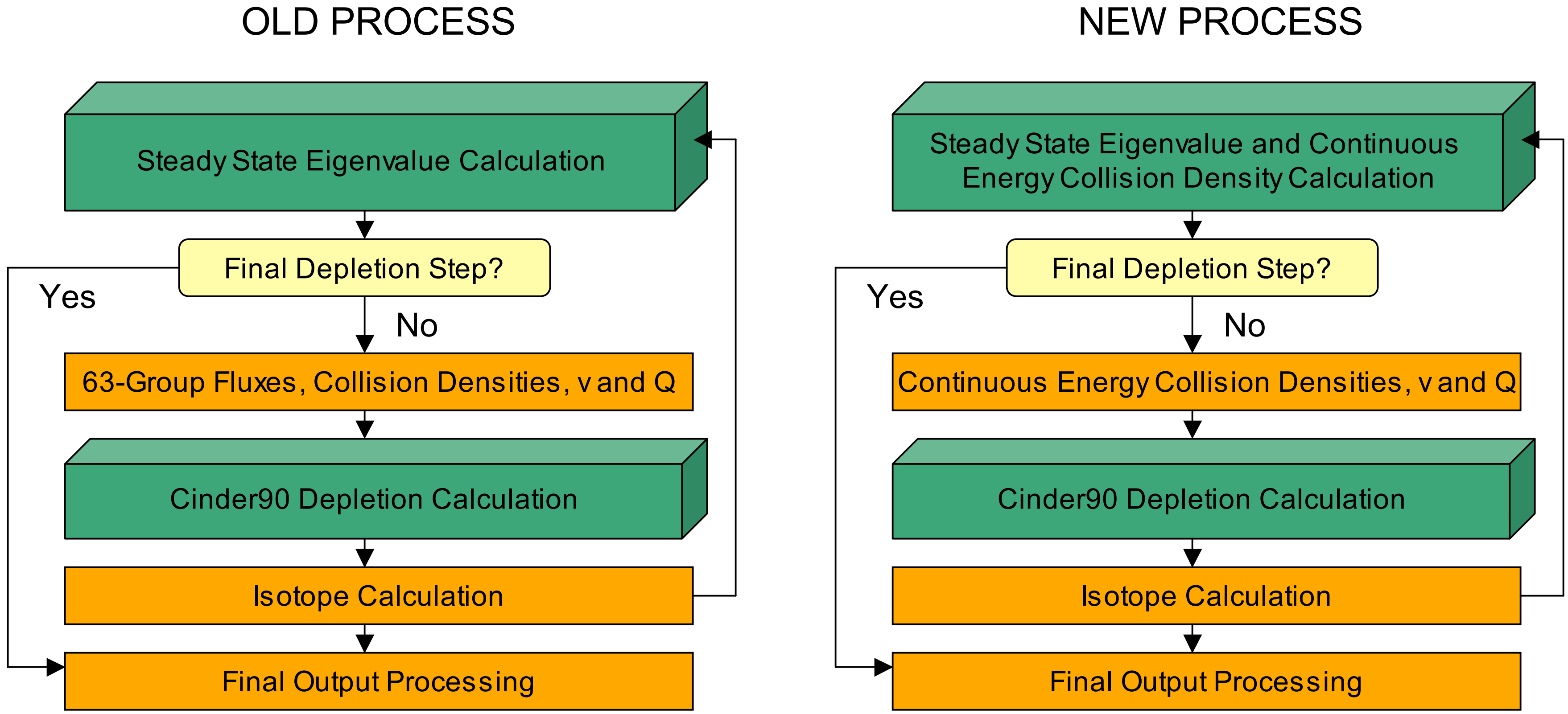
MCNPX: Accomplishments and Possibilities

FY05 + FY06 Q1: MCNPX Depletion Process

- Utilizes user defined time steps, power levels and varied power fractions
- Burns multiple materials and allows the user to omit certain isotopes from the depletion process
- Assumes constant flux approximation for depletion
- Runs with/without cross section models
- Prints individual material burnup and total system burnup as well as time dependant isotope concentrations at each burn step.

- Utilizes continuous energy collision densities for (n,γ), (n,f), (n,2n), (n,3n), (n,α) and (n,p) to generate one-group cross sections for CINDER90 depletion
- Generates fission products based on selected predefined fission product "Tiers"
- Tracks concentrations of all the possible daughters reactions from isotopes specified as burn materials utilizing isotope generator algorithm
- Automatic fission yield selection for depletion in CINDER90

MCNPX Depletion Process
Continuous Energy Collision Densities

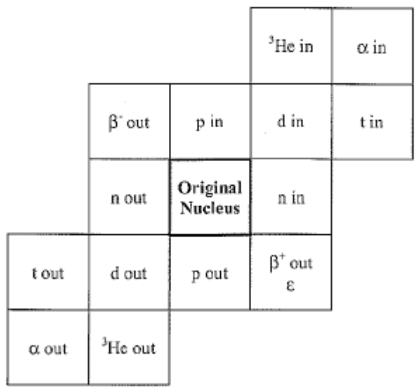


- MCNPX no longer generates 63-group collision densities by matching a 63-group Monte Carlo derived flux to 63-group cross sections inherent to CINDER90

MCNPX Depletion Process
Fission Product Tiers

- Certain Monte Carlo linked depletion codes force the user to input every fission product to be tracked during the depletion process
- MCNPX offers the user preset fission product "tier"s
- Eliminates the task of inputting every fission product to be tracked
- MCNPX offers three fission product tiers
  - Tier 1. (default) Zr-93, Mo-95, Tc-99, Ru-101, Xe-131, Cs-133, Cs-137, Ba-138, Pr-141, Nd-143, Nd-145
  - Tier 2. Isotopes contain in the fission product array that are included in the current cross section library file (XSDIR) for MCNPX version 2.6.A
  - Tier 3. All isotopes contained in the fission product array
- The user then has the option to eliminate certain isotopes from a tier if necessary

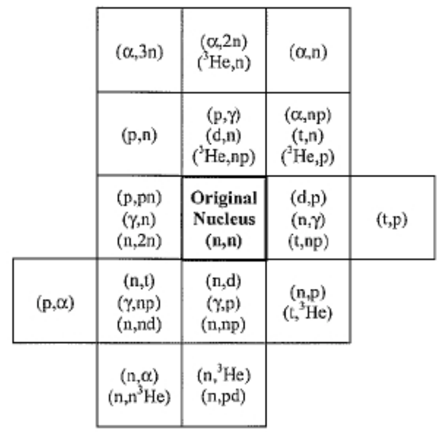
MCNPX Depletion Process
Isotope Generator Algorithm



n = neutron
p = proton
d = deuteron
t = triton

α = alpha particle
β^- = beta minus (negative electron)
β^+ = beta plus (positron)
ε = electron capture

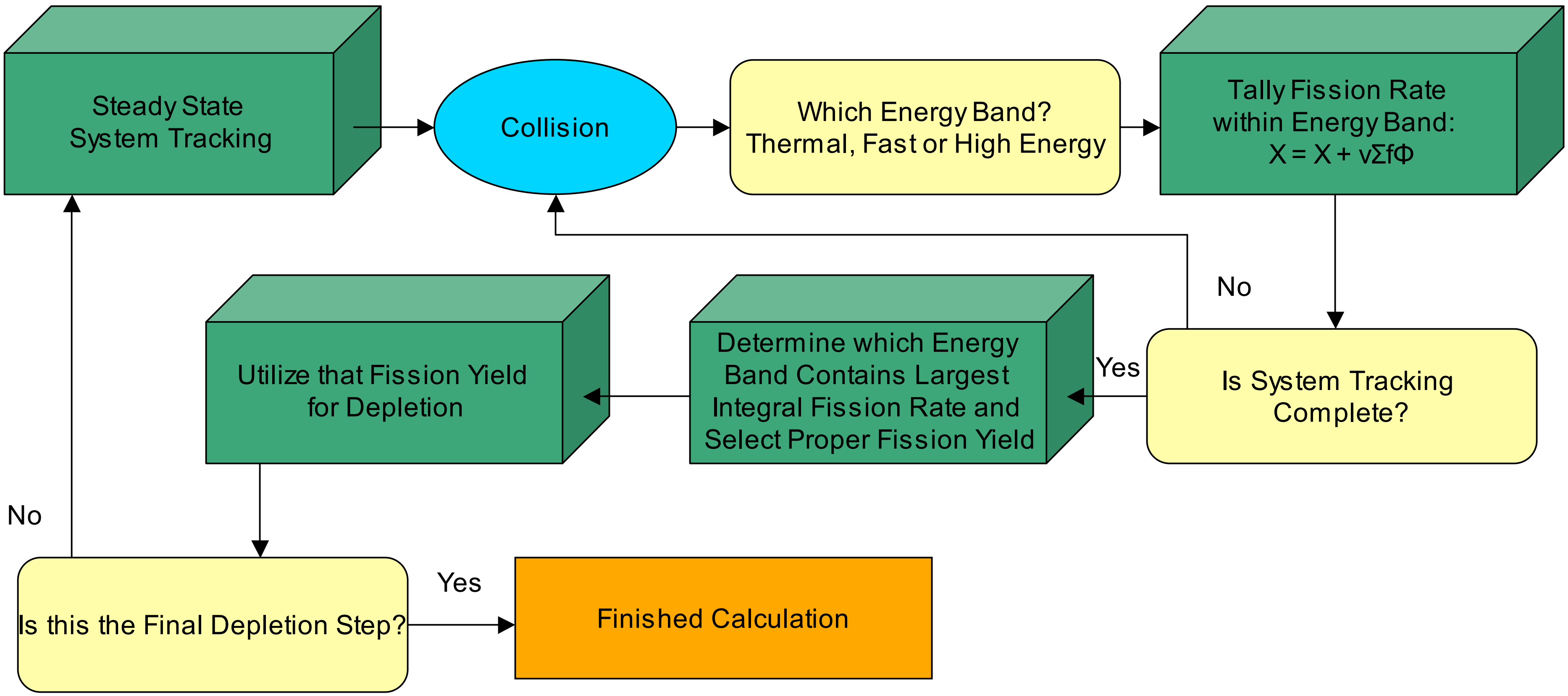
Relative Locations of the Products of Various Nuclear Processes on the Chart of the Nuclides.



Changes Produced by Various Nuclear Reactions.

- Capturing every possible decay chain product from every isotope generated during the depletion process would be extraordinarily memory intensive
- MCNPX utilizes the isotope generator algorithm to determine all the immediate daughter isotopes created from a burn material reaction, and tracks those isotopes during the transport process

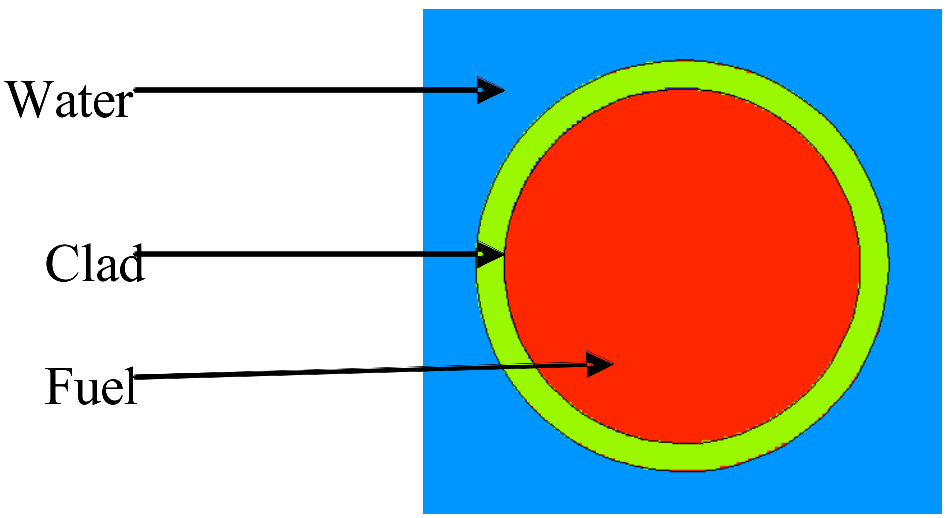
MCNPX Depletion Process
Automatic Fission Yield Selection



- Automating the fission yield selection process eliminate computational cost associated with preliminary neutron spectrum calculation

MCNPX Depletion Process Benchmark Calculation

Infinitely reflected MOX pin cell geometry with borated water



Fuel Composition

ZAID	Atom Fraction
8016.60c	4.59E-02
92235.60c	1.45E-04
92238.60c	1.99E-02
94238.60c	1.15E-04
94239.60c	1.03E-03
94240.60c	7.97E-04
94241.60c	3.40E-04
94242.60c	5.64E-04

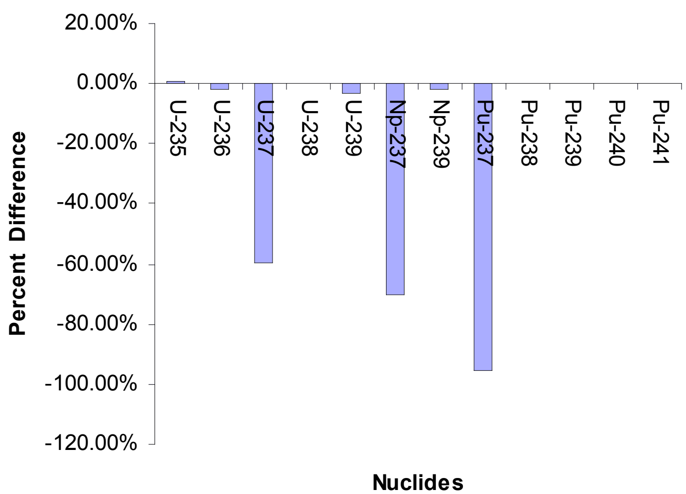
Water Composition

ZAID	Atom Fraction
1001.60c	4.77E-02
8016.60c	2.39E-02
5010.60c	3.63E-06
5011.60c	1.62E-05

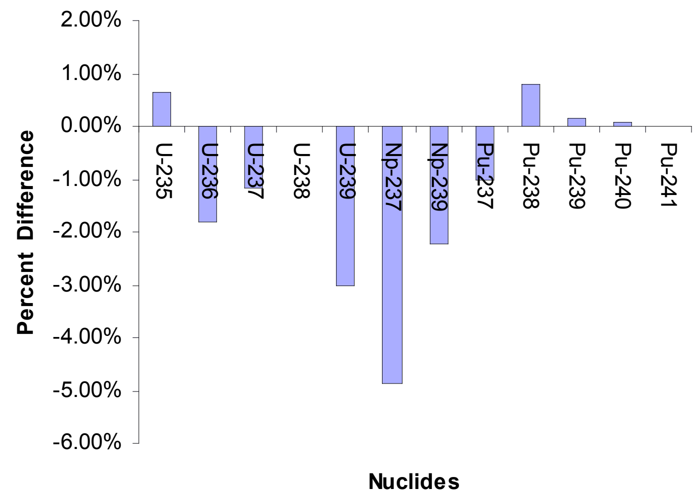
- The fuel pin was depleted at a power of 66.956 kWt over the time durations of 0.645 days, 40 days, 100 days, 140 days, 200 days, and 250 days for a total of 730.645 days (2 years).
- Depleting utilizing MONTEBURNS, old MCNPX and new MCNPX

Comparison of EOL Actinide Masses
MCNPX vs. MONTEBURNS

Old MCNPX



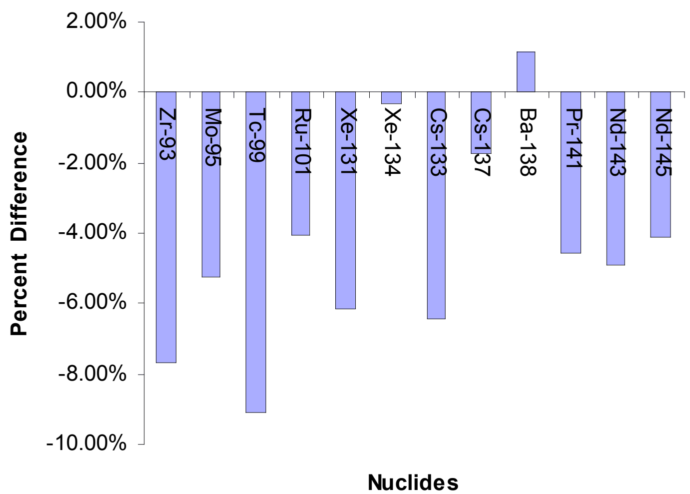
New MCNPX



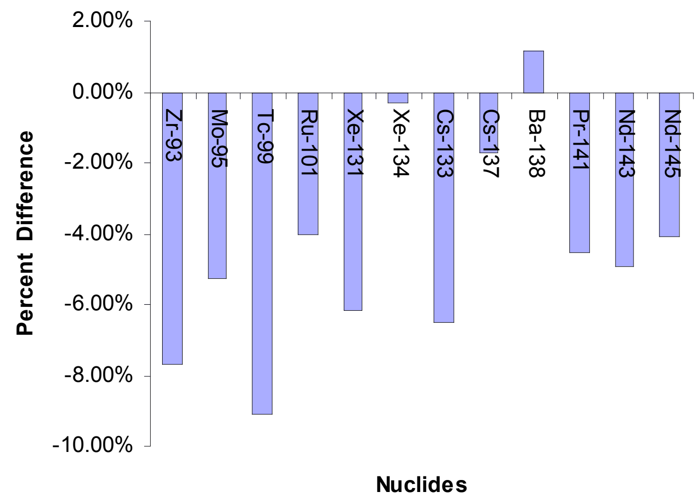
- Adding continuous energy collision densities decreases the percent difference between MCNPX and MONTEBURNS
- The minimal percent difference (<5%) still exhibited is a due to lack of predictor corrector methodology

Comparison of EOL Fission Product Masses MCNPX vs. MONTEBURNS

Old MCNPX



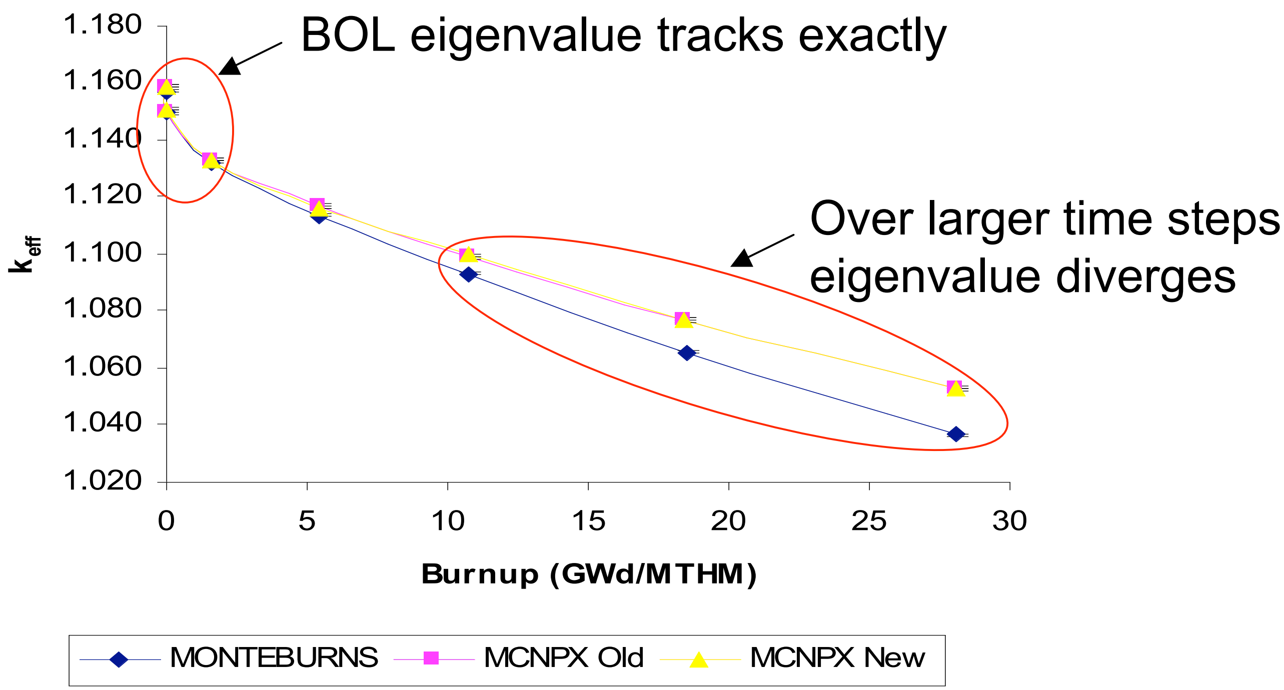
New MCNPX



- Adding continuous energy collision densities has no effect on the percent difference between MCNPX and MONTEBURNS
- The minimal percent difference (<10%) still exhibited is a due to lack of predictor corrector methodology and possible differences in the fission yields from the inherent libraries in each depletion code

MCNPX: Accomplishments and Possibilities

Need for Predictor Corrector



- Eigenvalue of MCNPX diverges from MONTEBURNS over large time steps
  - Different yield data
  - Absence of predictor corrector technology

MCNPX Depletion Process: Summary

- MCNPX allows complete, relatively easy-to-use depletion calculations in a single Monte Carlo code
- Input is simple, and the output is highly organized
- Automated features decrease the amount of necessary user input to achieve a reliable answer
  - Fission Product Tiers
  - Isotope Generator Algorithm
  - Automatic Fission Yield Selection
- The current version of MCNPX benchmark's well against MONTEBURNS
  - Continuous energy collision densities corrected actinide production problems
  - Minimal differences are exhibited
    - Lack of Predictor Corrector
    - Possible discrepancies in yield libraries
- Development of linear predictor corrector is underway along with further improvements to enhance the usefulness of this new capability.

MCNPX: Accomplishments and Possibilities

FY06 Milestones:

- AFCI: Implement predictor/corrector step for CINDER'90 burnup module in MCNPX *0.25 FTE*
    - code maintenance / documentation; **V26A**
    - release of code versions with new capabilities / SQA;
    - user training / workshops / support;
    - research into correct flux / source distributions in near-critical systems in collaboration with Purdue University.
- MTS: CEM03 / LAQGSM *0.4 FTE*
- GEN-IV: none
- Other: MCNPX/MCNP merger

MCNPX: Accomplishments and Possibilities
Workshops

- **FY05:**
  - Las Vegas
  - Mol (Belgium)
  - Santa Fe(2)
  - Seoul (Korea)
- **FY06**
  - January - Las Vegas
  - March – Cape Town (South Africa)
  - May – Santa Fe
  - July – London (England)
  - September – Santa Fe

MCNPX: Accomplishments and Possibilities
Workshops

MCNPX: Accomplishments and Possibilities

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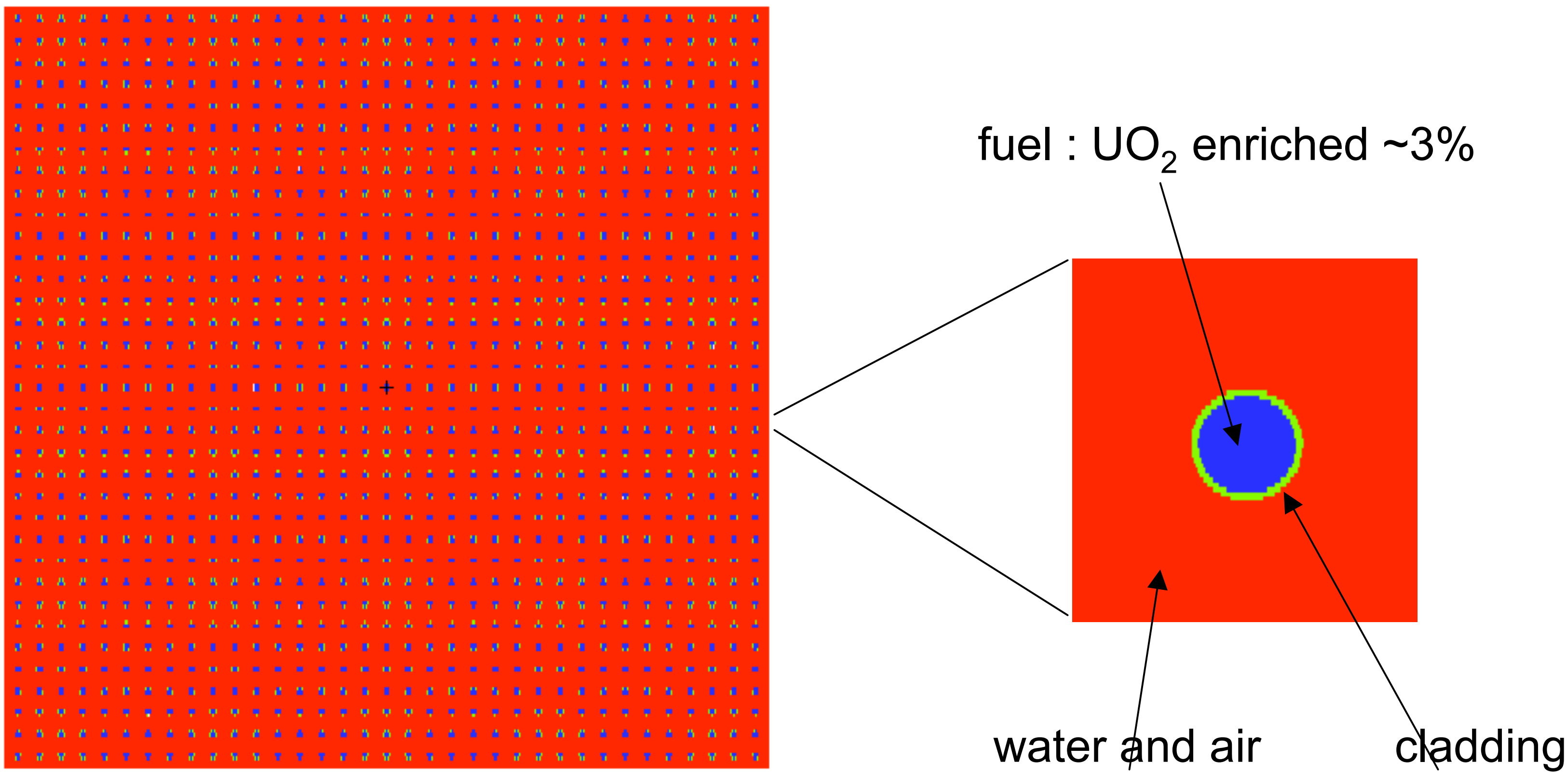
MCNPX: Accomplishments and Possibilities

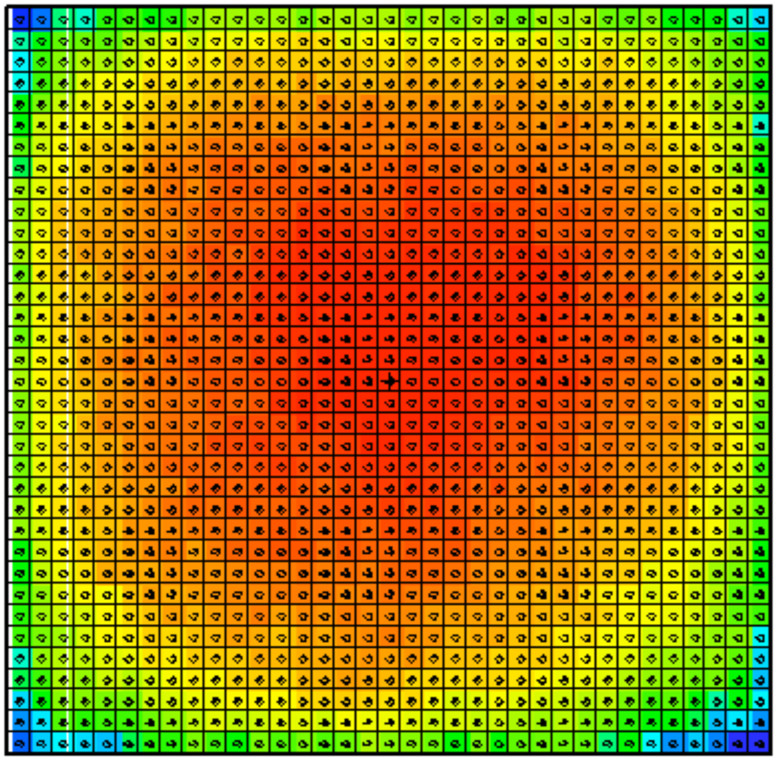
Correct Flux Distributions in Near-Critical Systems



35 X 35 lattice of fuel pins : 330 cm long, 0.8cm radius
Bad initial source distribution : bottom left quadrant 3
10 inactive cycles, 40 active, 1000 histories/cyc.

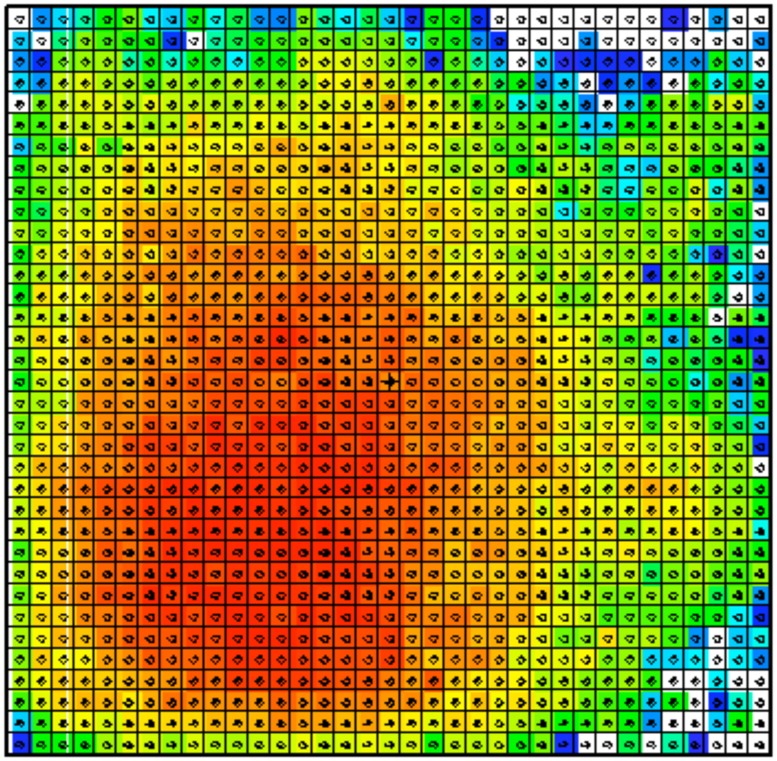
MCNPX: Accomplishments and Possibilities

Correct Flux Distributions in Near-Critical Systems



"Converged" with Standard Monte Carlo

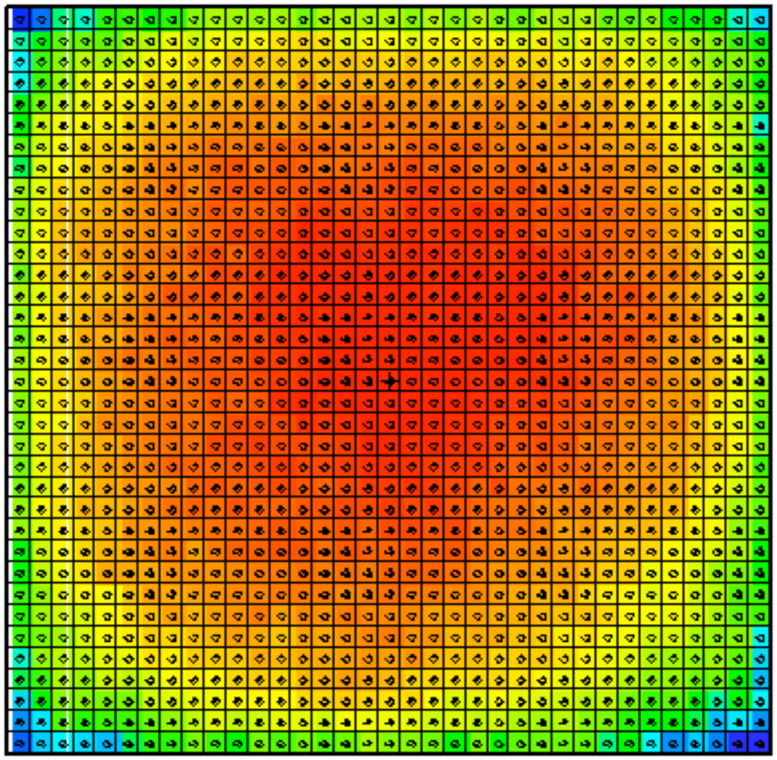
MCNPX: Accomplishments and Possibilities
Correct Flux Distributions in Near-Critical Systems



50 thousand histories with Standard Monte Carlo
faulty initial source distribution still apparent

MCNPX: *Accomplishments* and Possibilities

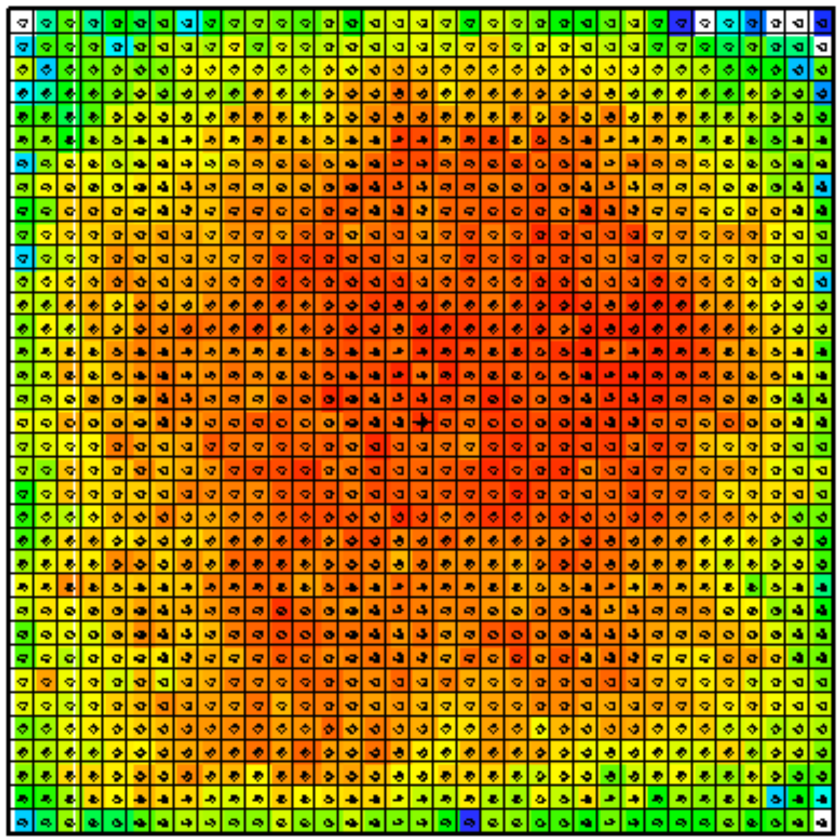
Correct Flux Distributions in Near-Critical Systems



“Converged” with Standard Monte Carlo : 1 million histories

MCNPX: Accomplishments and Possibilities

Correct Flux Distributions in Near-Critical Systems



50 thousand histories with Vacation Matrix
method
recovered from faulty initial source distribution

MCNPX: Accomplishments and Possibilities

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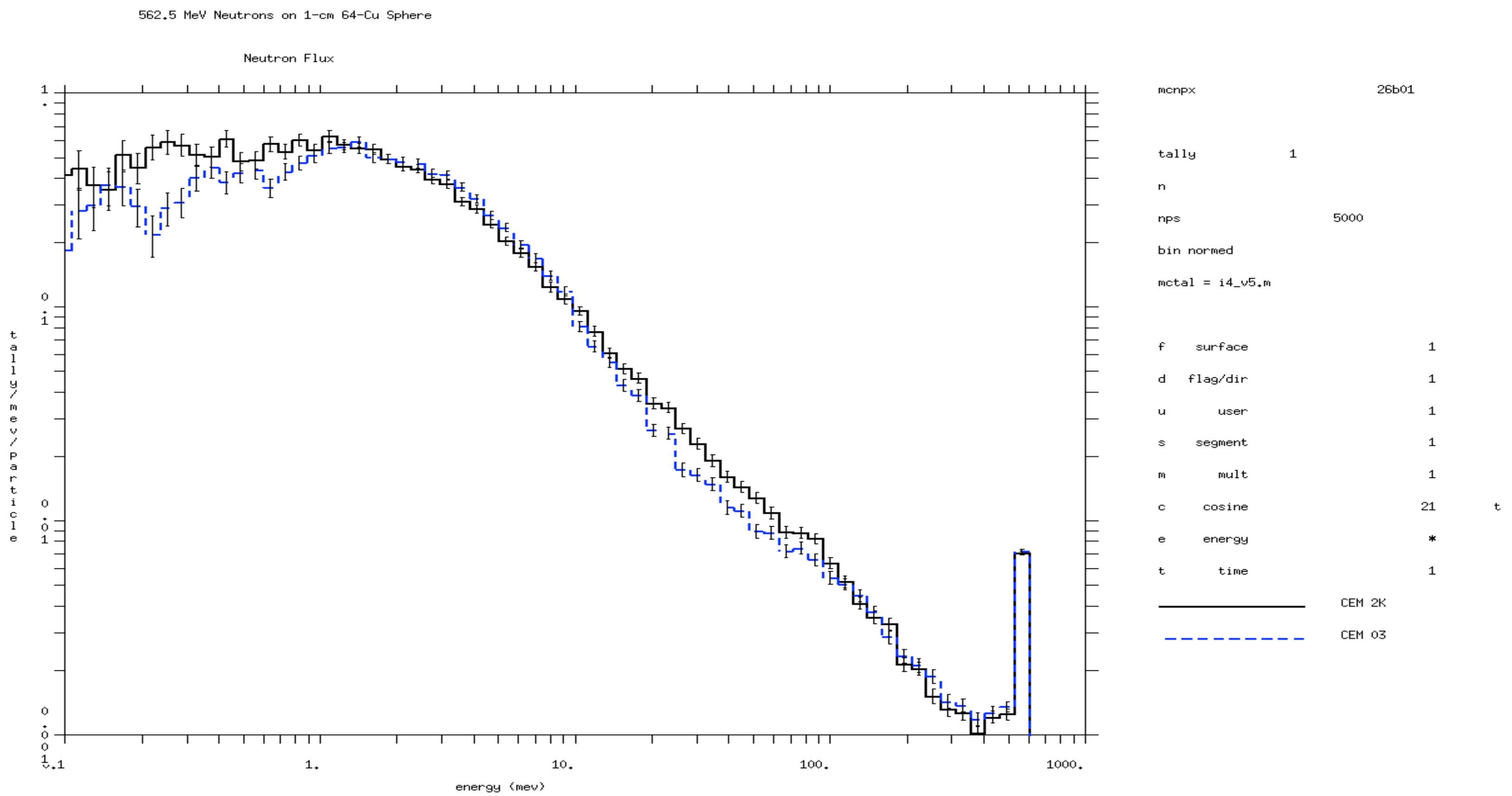
MCNPX: Accomplishments and Possibilities
MTS: CEM03 / LAQGSM

- Convert stand-alone CEM03 / LAQGSM code to F90 module;
- Develop and match test problems;
- Modify MCNPX and insert CEM03 module;
- Match match test problems;
  - *Accomplished January 20, 2006 (last Friday)*
- *Integrate module – plotters, parallelization, etc.*
- *Integrate LAQGSM capability*

MCNPX: Accomplishments and Possibilities

MTS: CEM03 / LAQGSM



MCNPX: Accomplishments and Possibilities

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MCNPX/MCNP Merger

- *August 2005: memorandum of understanding*
- *October 2005: X-Division reorganization*
- *December 2005: meet with PADWP / X-Div*
- *December 2005: MCNPX to X-Div proposal with deliverables, milestones, funding request*
- *January 2006: verbal acceptance*
- *January 2006: RSICC release of combined MCNP5 / MCNPX / Data package*
- *February 2006: coordination board, procedural, and*
- *SQA review and protocols*
- *March 2006: begin feature migration*

MCNPX: Accomplishments and Possibilities
MCNPX Depletion Process

- Implementing accurate predictor corrector methodology (FY06)
  - *Approximate an average flux over the entire burn step*
  - *Consider more sophisticated approaches*
- Variable materials: making geometry perturbations during the burnup calculation
- Continued integration: Plotting, user features, etc.

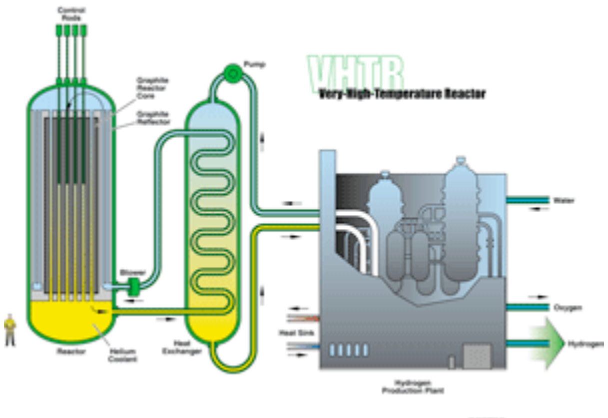
- Accurate Q value tracking
  - Neither MCNPX nor ENDF Q values include delayed gamma contribution
  - Since the Q value is underestimated the flux multiplier is overestimated and thus the flux is over estimated
  - Since flux is overestimated, burnup is over estimated
- Calculating number density error and error propagation during the depletion process
  - Toshikazu Taked, Naoki Hirokawa and Tomohiro Noda "*Estimation of Error Propagation in Monte-Carlo Burnup Calculations*" Journal of Nuclear Science and Technology, Vol 36, No. 9, September 1999.
- Automatic burn step generation
  - Determine the placement of the minimal amount of burn steps in order to achieve a reliable answer

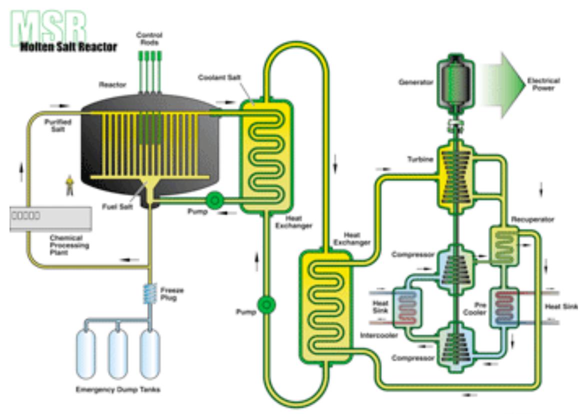
MCNPX: Accomplishments and Possibilities
More Worthy Proposals

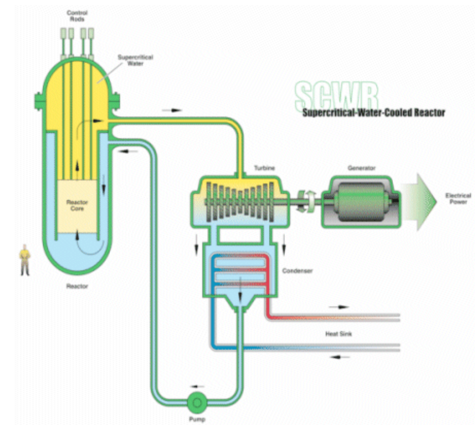
- *Continue INCL collaboration*
- *Continue Purdue collaboration*
- *Reinstate IM-8 participation*
- *Continue maintenance and user support*
- *Better integrate recent capabilities*
  - *INCL*
  - *CEM03/LAQGSM*
  - *Mesh tally plotting*
  - *CINDER90 / burnup*

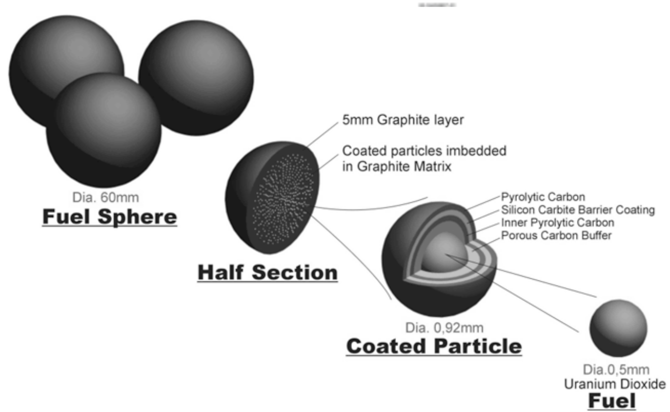
MCNPX: Accomplishments and Possibilities

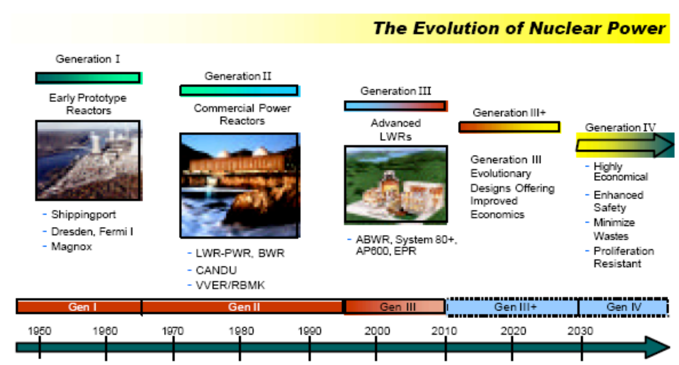
Generation IV Reactor Core Modeling











- As advanced reactor concepts challenge the accuracy of current modeling technologies, a higher fidelity more robust transport / depletion tool is necessary in order to properly model time-dependant core characteristics

AFCI and MCNPX
Funding History

- ***FY01 – 4 FTE ? (LSW / HGH / JSH / GWM, IM-8)***
- ***FY04 - $300K***
- ***FY05 - $250K*** *~ .6 FTE*
- ***FY06 - $275K*** *– 3% of $7M program*

  FY06 CR - $100K *– 2% of $5M program*

  ~ .23 FTE ~ 11 weeks

- At the very least, we need help securing GEN-IV funding

AFCI and MCNPX

Devastation:

- *IM-8 build system / computer infrastructure stalled;*
- *Purdue student let go;*
- *Laurie Waters turned away;*
- *May abandon CEA / Saclay INCL4 / ABLA collaboration;*
- *JSH has taken 6 month half-time assignment.*

JUSTIFICATION

- What's the point of measuring and evaluating cross sections and other data if it kills the code that uses them?
- Is 70% data / 3% codes a good balance?
- MCNPX is used across AFCI program;
- AFCI is the *fulcrum* of MCNPX leveraged development;
  - *Maintenance, users, documentation, students, IM-8 computations, distribution, modernization, corrections …*
- MCNPX has 2 of 6 transmutation physics level 2 milestones for FY06;
- Commitments to CEA/Saclay (INCL4/ABLA);
- Track record of delivering excellence.